Multiresolution computing platform for nuclear energy density functional

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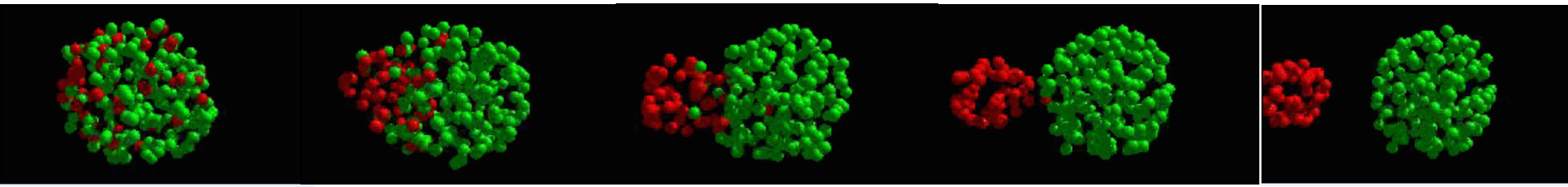
Supported by DOE's SciDAC UNEDF Project

CScADS 2009 Workshop, Tahoe, CA

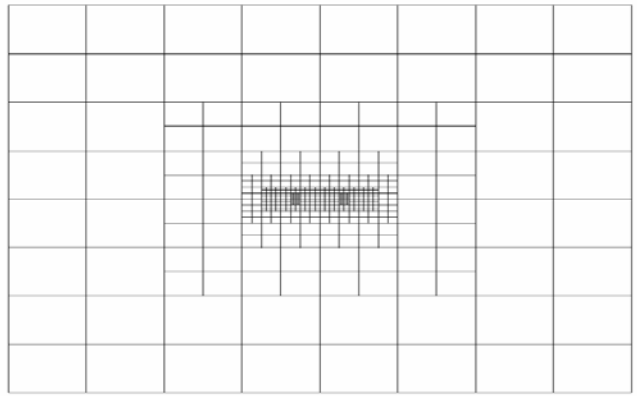
Nuclear EDF computing

- *Most nuclear physics codes are based on the HO basis expansion method. Precision not guaranteed in case of weakly-bound or very large deformations.*
- *Not suitable for leadership computing, not easily parallelizable*
- *2D coordinate-space Hartree-Fock-Bogoliubov code was based on B-Spline techniques: HFB-AX*
- *3D coordinate-space HFB is not available. Developing MADNESS-HFB*
- *Applications: complex nuclear fission, fusion process.*



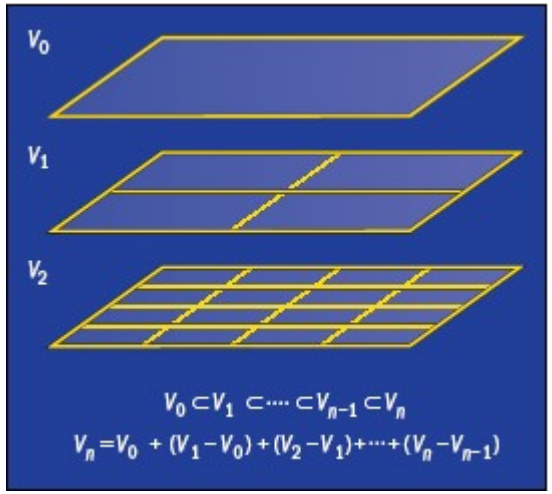
MADNESS

- ***M**ultiresolution **AD**aptive **N**umerical **E**nvironment for **S**cientific **S**imulation*
- *A collaborative endeavor of mathematics (George Fann) and computational chemistry (Robert Harrison)*
- *Computing using leadership-class supercomputers: high-precision, scalable, portable*
- *Applications include: chemistry, atomic and molecular physics. material science, and **nuclear structure**.*



Mathematics

- Multiresolution



- Approximation using Alpert's multiwavelets

Function represented by 2 methods:
1.scaling function basis
2. wavelet basis.

$$f^n(x) = \sum_{l=0}^{2^n-1} \sum_{i=0}^{k=1} s_{il}^n \phi_{il}^n(x)$$

$$f^n(x) = \sum_{i=0}^{k-1} s_{i0}^0 \phi_{i0}^0(x) + \sum_{n=0\ldots} \sum_{l=0}^{2^n-1} \sum_{i=0}^{k=1} d_{il}^n \psi_{il}^n(x)$$

- Low-separation rank: (e.g., optimized approx of Green functions with Gaussians, Beylkin-Mohlenkamp, Harrison)

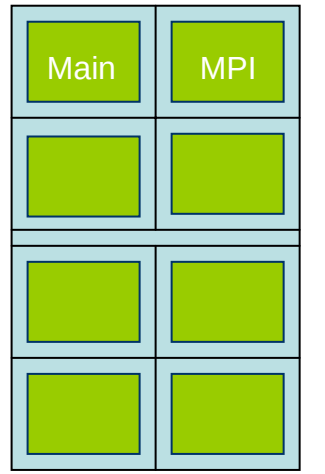
$$f(x_1, \ldots, x_n) = \sum_{l=1}^{M} \sigma_l \prod_{i=1}^{d} f_i^{(l)}(x_i) + O(\epsilon)$$

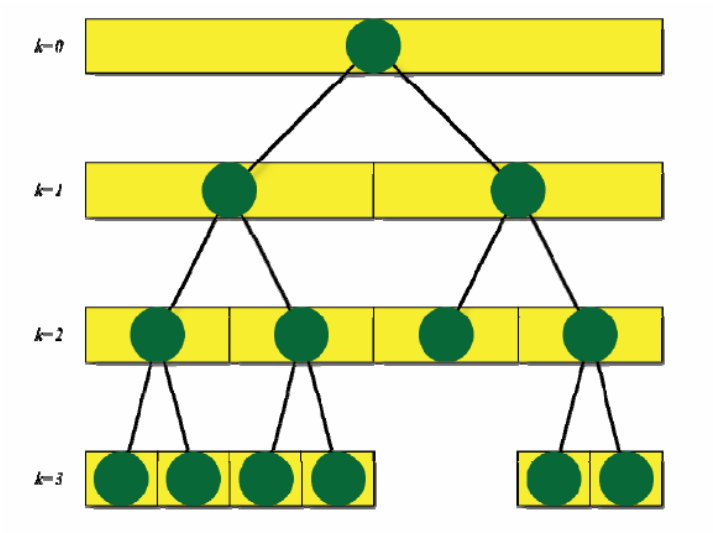
$$\left\| f_i^{(l)} \right\|_2 = 1 \qquad \sigma_l > 0$$

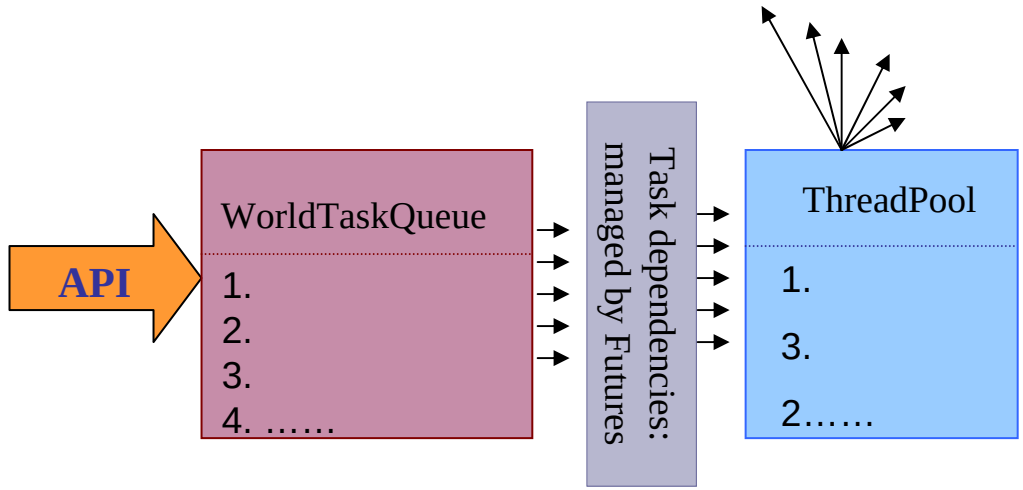
Parallel computing strategy

- MPI: node to node communication
- Distributed arrays and FUTURES
- Pthreads: multi-threading within one node

  threads per node: 6+main+server = 8
- Load-balance: map tree to parallel hash table







Solving Schrodinger Equation

Solving Schrödinger Equation (integral form, Kalos):

$$\left(-\tfrac{1}{2}\nabla^2 + V\right)\Psi = E\Psi$$

$$\Psi = -2\left(-\nabla^2 - 2E\right)^{-1} V\Psi$$

$$= -2G*\left(V\Psi\right)$$

$$\left(G*f\right)(r) = \int ds \frac{e^{-k|r-s|}}{4\pi|r-s|} f(s) \quad \text{in 3D} \; ; \; k^2 = -2E$$

Approximate the bound-state Helmholtz operator $\dfrac{e^{-\mu r}}{r}$ using Gaussians:

- Spin-orbit coupling implemented in nuclear physics

Solving HFB

Superfluidity with pairing

$$\begin{pmatrix} h(\boldsymbol{r})-\mu_{\uparrow} & \Delta(\boldsymbol{r}) \\ \Delta^{\dagger}(\boldsymbol{r}) & -h(\boldsymbol{r})+\mu_{\downarrow} \end{pmatrix} \begin{pmatrix} u_i(\boldsymbol{r}) \\ v_i(\boldsymbol{r}) \end{pmatrix} = E_i \begin{pmatrix} u_i(\boldsymbol{r}) \\ v_i(\boldsymbol{r}) \end{pmatrix}$$

Particle number condition

$$N_{\uparrow} = \sum_{-E_{cut}<E_i<0} \int |u_i(\mathbf{r})|^2$$

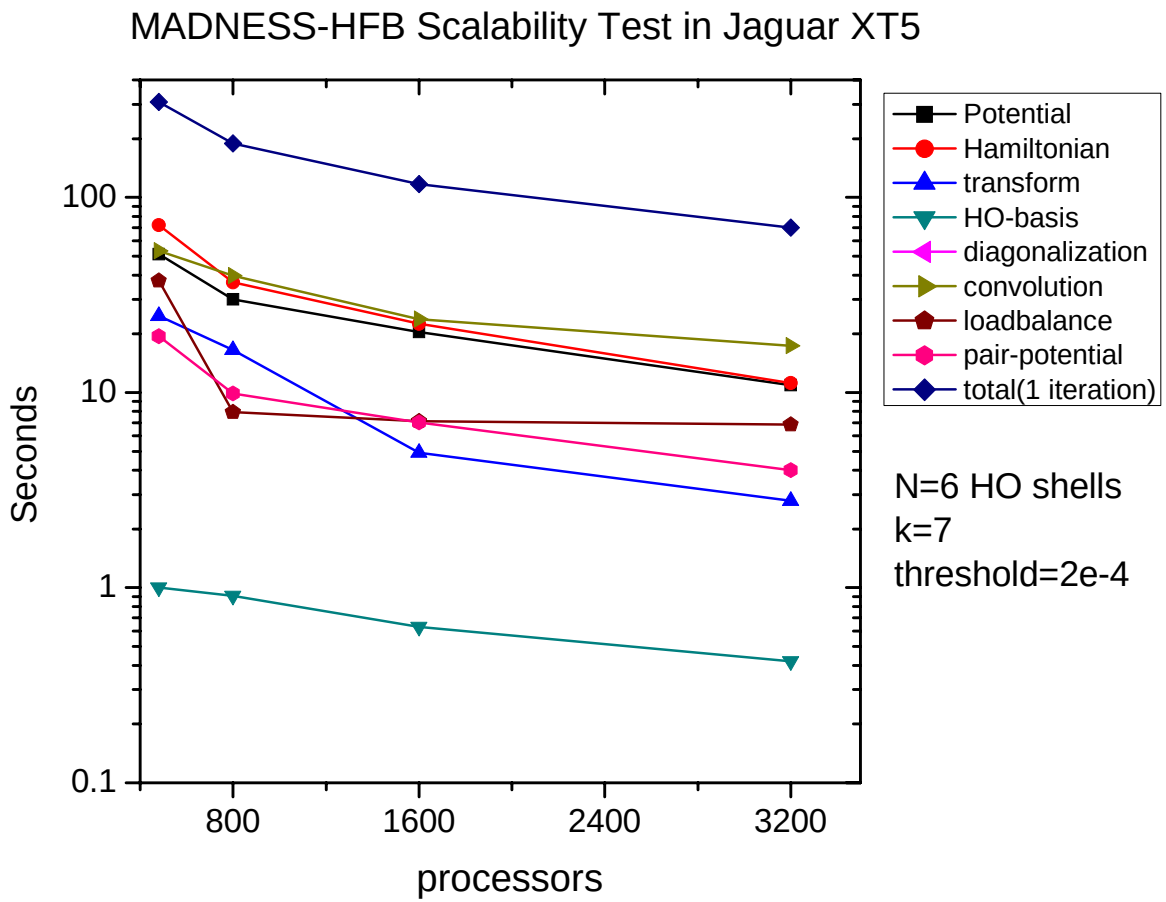
$$N_{\downarrow} = \sum_{0<E_i<E_{cut}} \int |v_i(\mathbf{r})|^2$$

- Initial guess Wavefunctions
- Construct Hamiltonian
- Diagonalization
- Improve approximations by applications of BS Helmholtz kernel
- Iteration until convergence

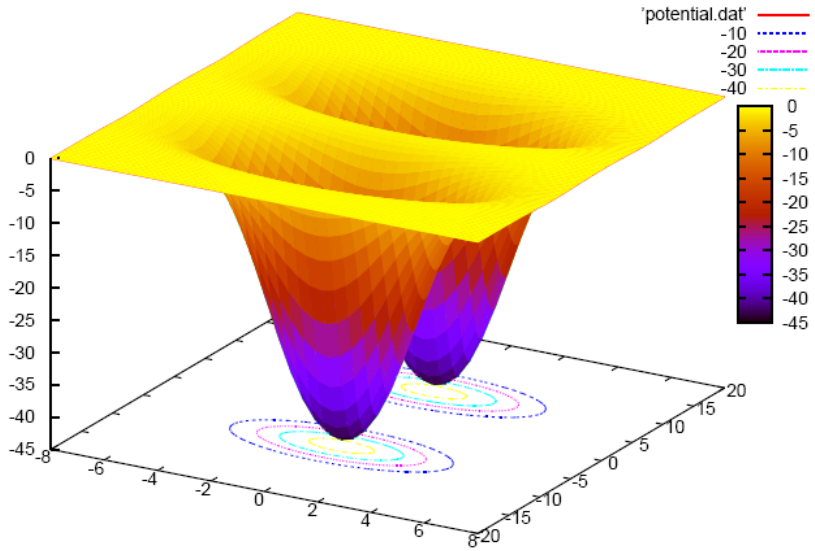
SLDA density functional:

$$\mathcal{E}(\mathbf{r}) = \alpha\frac{\tau_c(\mathbf{r})}{2} + \beta\frac{3(3\pi^2)^{2/3}n^{5/3}(\mathbf{r})}{10} + g_{\mathit{eff}}(\mathbf{r})|\nu_c(\mathbf{r})|^2 + V_{ext}(\mathbf{r})n(\mathbf{r}),$$

HFB (prelim, 8/2/2009)



Two-cosh potential test



Precision Test with spin-orbit

State No.	Ω^π	HO N_{sh}=20	HO N_{sh}=30	B-spline h=0.6	Wavelets
1	$1/2^+$	−22.23916	−22.24008	−22.24011	−22.24011
2	$1/2^-$	−22.23816	−22.23995	−22.23998	−22.23998
3	$1/2^+$	−9.43145	−9.43659	−9.43663	−9.43662
4	$3/2^-$	−9.42314	−9.43199	−9.43203	−9.43202
5	$3/2^+$	−9.42561	−9.43078	−9.43081	−9.43080
6	$1/2^-$	−9.41931	−9.42783	−9.42788	−9.42788
7	$1/2^+$	−8.77250	−8.77825	−8.77828	−8.77828
8	$1/2^-$	−8.76475	−8.77380	−8.77384	−8.77383
9	$1/2^+$	−1.70727	−1.72405	−1.72506	−1.72516
10	$1/2^-$	−1.49222	−1.52490	−1.52675	−1.52693

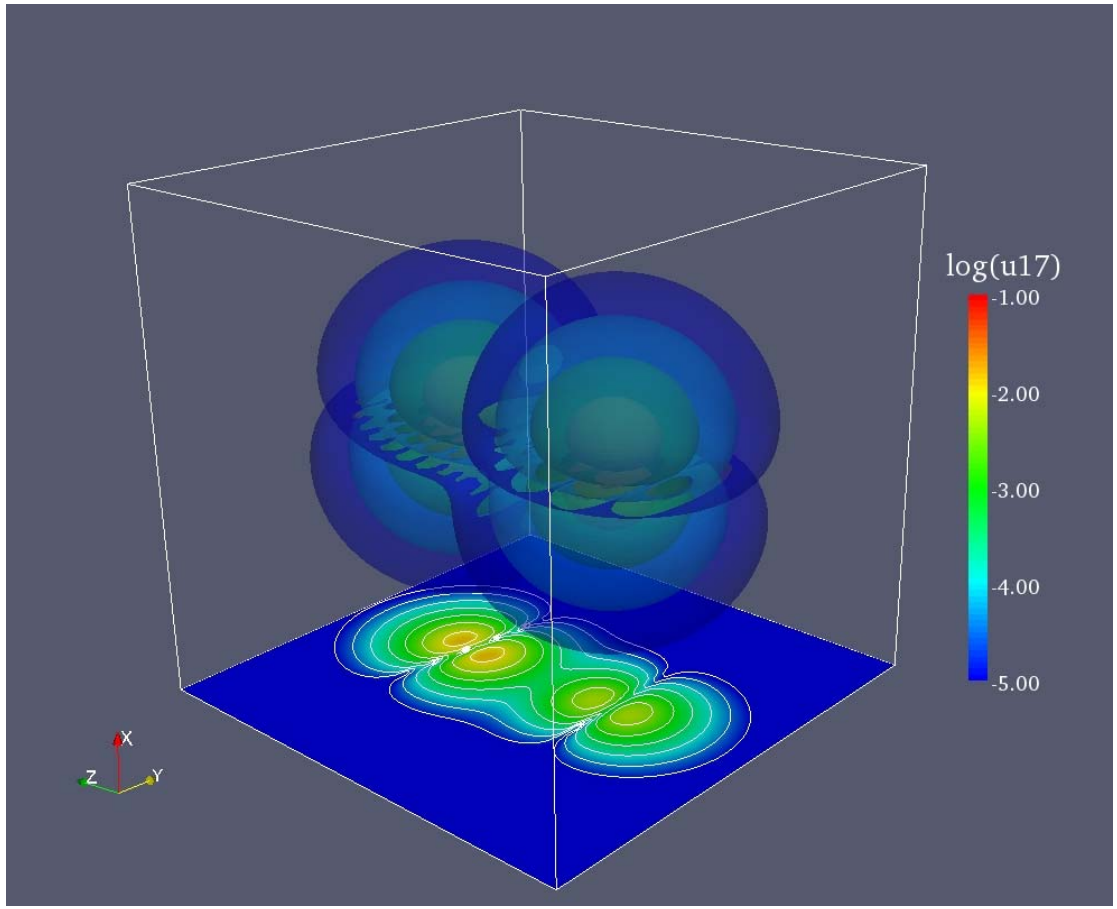
- Similar to nuclear fission problem

$$V_{so} = -\sqrt{-1}\lambda_0 \left(\frac{h}{2mc}\right)^2 \nabla V \bullet (\sigma \times \nabla)$$

$$h = -\frac{\hbar^2}{2m}\nabla^2 + V_{2\cosh}(x, y, z) + V_{so}(x, y, z)$$

Visualization

- VTK-paraview A wavefunction example



Outlook

1. Target is to develop an accurate, scalable, portable 3D nuclear DFT solver. Preliminary two-cosh potential tests have done.
2. HFB solver with bound-state solutions has been implemented.
3. Outgoing boundary condition is being developing to describe continuum effects and resonance states.

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Thanks

- Robert Harrison.
- Judith Hill for the 3-D orbit VTK code and plots.